DTO CB.42
Environmental Fate of Agents

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AGENTFATE

Objectives:

- Measure and understand the physico- chemical processes of CW agents on surfaces in order to predict their persistence and fate in operational scenarios via agent fate models.

Payoffs:

- Support research and acquisition decisions of all capability areas: detection, protection, decontamination
- Support and improve Operational Risk Management decisions based on inhalation and contact hazard.
- JFOC - Battle Management: Battlespace Analysis and Planning
- Augments operational and mission area analysis tools such as Joint Effects Model (JEM) and Joint

SUMMARY ACCOMPLISHMENTS AS OF 2003 TARA

- Field testing from 1999-2001 demonstrated that a comprehensive data collection and model enhancement effort was required to improve CW agents hazard prediction tools
- 2000/2001 field tests documented and published
- Expert analysis of agent fate and effects literature delivered
- CW agents synthesized and characterized; test surfaces identified
- Converted surface evaporation database to Oracle and added additional wind tunnel and field experiment data

Challenges: Developing a cost effective experimental design

- Complex set of surfaces, agents, and environmental conditions to measure
- Understanding scaling; Lab → Wind Tunnel → Field
- Dispersing multiple small thickened agent droplets
- Predictive modeling accuracy – limited CW agents outdoor field test facilities

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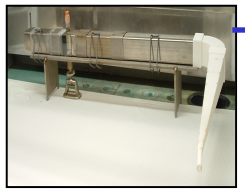
CONCEPT AND APPROACH

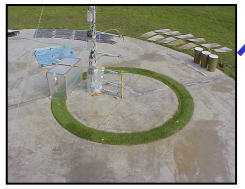
Three Major Thrusts

1 Methodology Development

- NMR
- HS-SPME
- Sand

Understanding of Agent/ Surface Chemistry





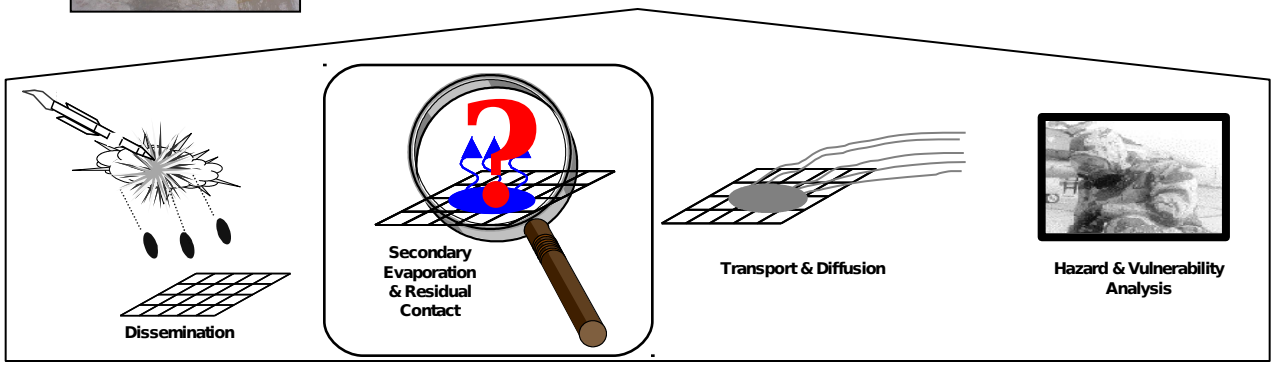
2 Lab/Wind Tunnel/Field Trials

- Surface Evaporation
- Substrate Interactions

vapor flux, temp., wind, RH, agent, substrate, drop size, spread rate, etc.)

3 Predictive Modeling

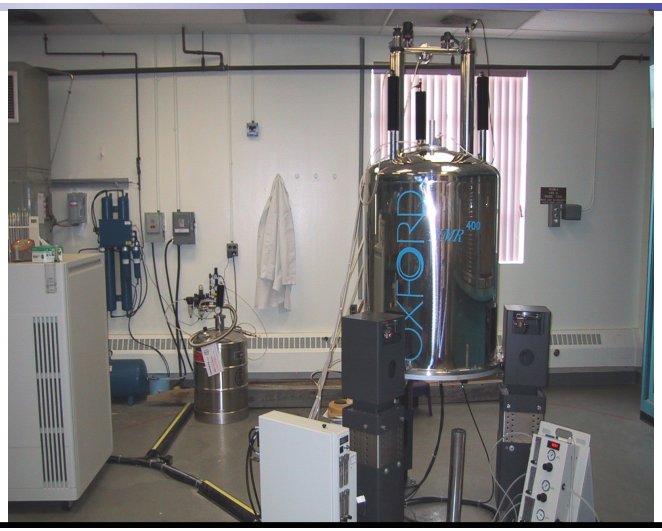
- Surface Evaporation and contact Database/ Modules
- CHEMRAT

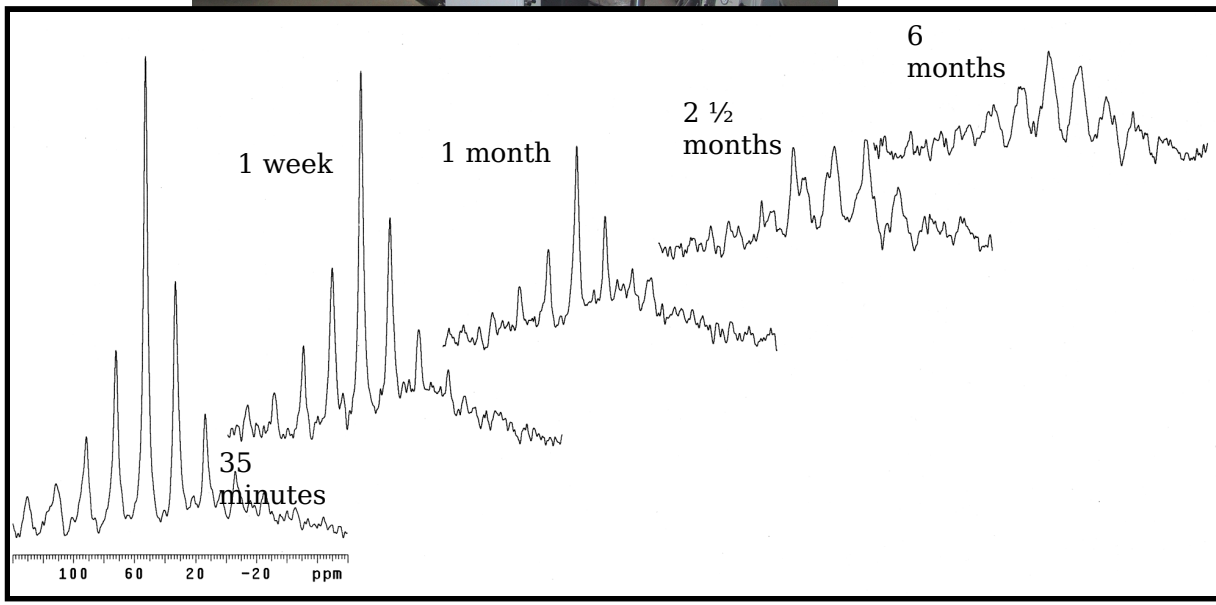


Operational Environment

Thrust: Methodology Development

- Determined VX fate on concrete by NMR
  - Rate fast and slow
  - Product no EA2192
  - Ethyl Methyl phosphonic acid
  - VX thiol
- Optimized / Validated HS-SPME technique
- Mass balance demonstrated with concrete, asphalt + soil
- Developed thickened agent formulation





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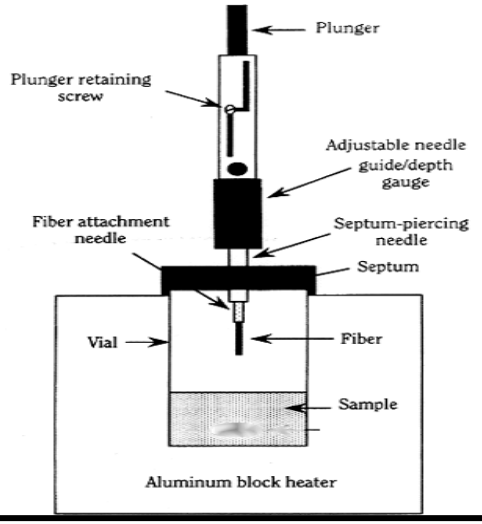
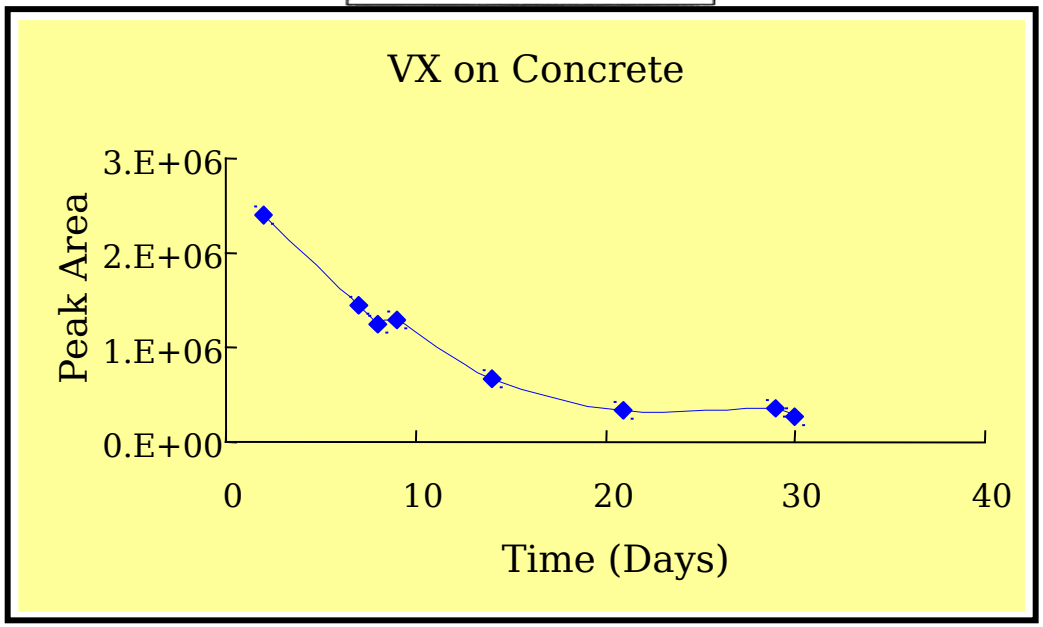
Thrust: Methodology Development

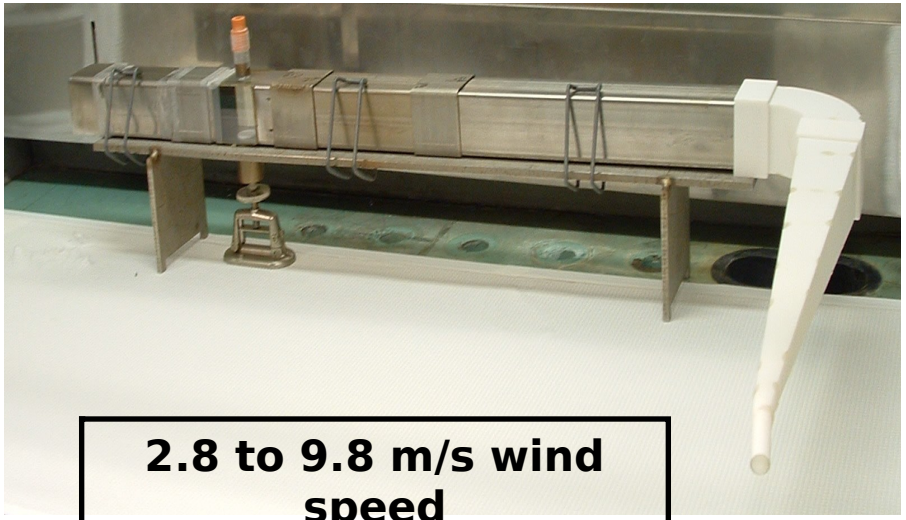
- VX, GD, and HD on four substrates by HS-SPME
- ECBC TR on HS-SPME technique available for review
- HD on concrete by NMR
- Develop soil system units &chamber sampling systems
- Control thickened agent deposition





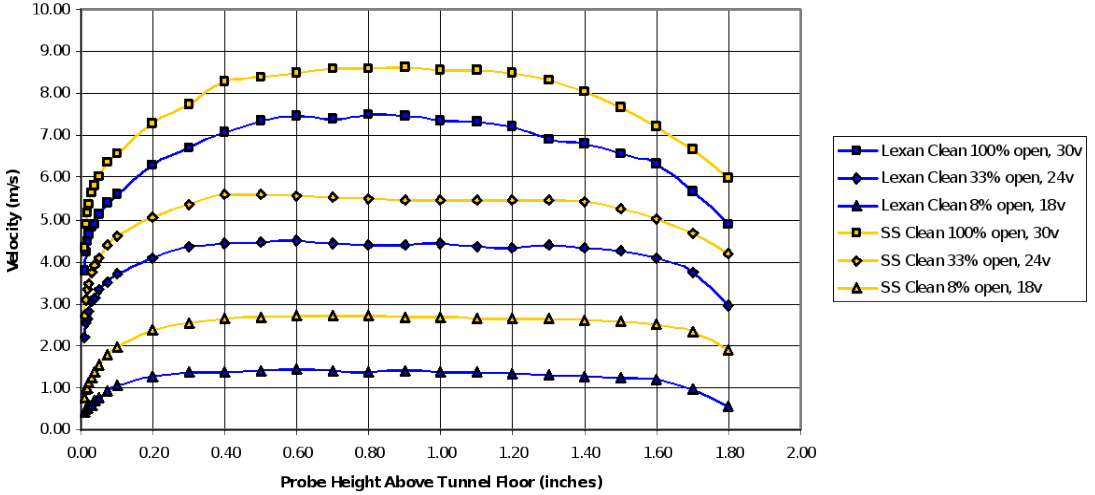
Thrust: Lab/Wind Tunnel Data

- ~~Per review panel~~ recommendation reoriented near term work from field testing to lab wind studies
- Measured surface evaporation of field tested HD on glass (outdoor)
- Designed and validated wind tunnel configurations



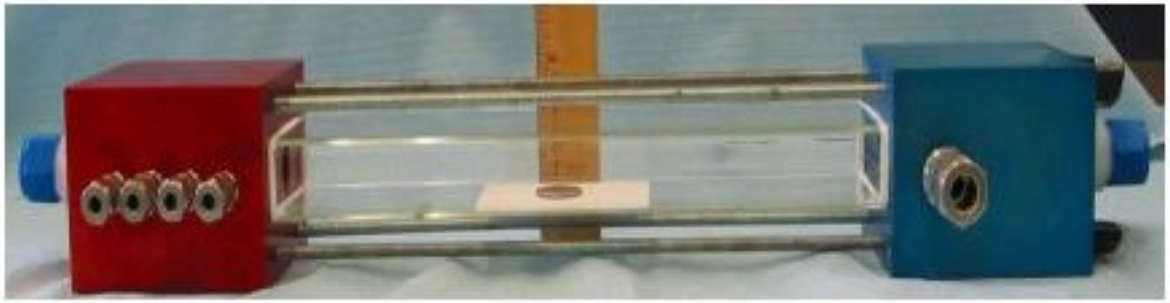
2.8 to 9.8 m/s wind speed

For Lexan and Stainless Steel Wind Tunnels



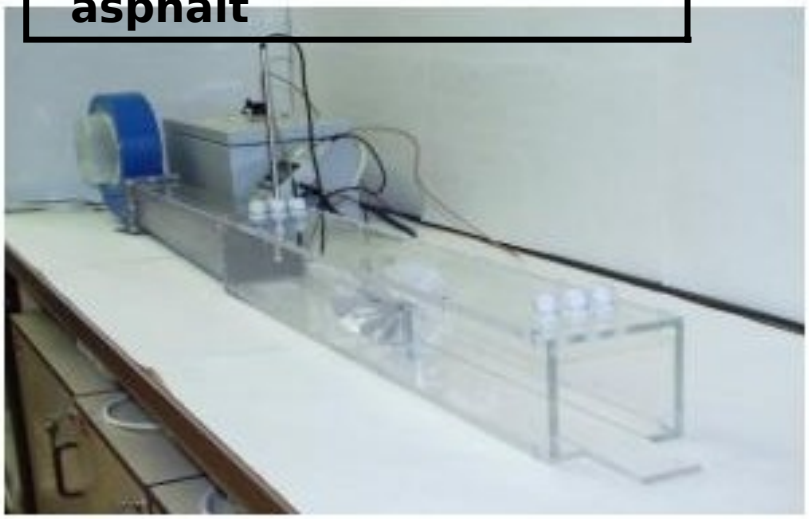
Thrust: Lab/Wind Tunnel Data

- Document &validate lab scale wind tunnels, HD on Aluminum
- Determine surface evaporation of HD & GD on concrete & begin asphalt



Length 30cm, Width 7.5cm, Height 2.6cm

Length 100cm, Width 5cm, Height 5cm



Length 100cm, Width 10cm, Height

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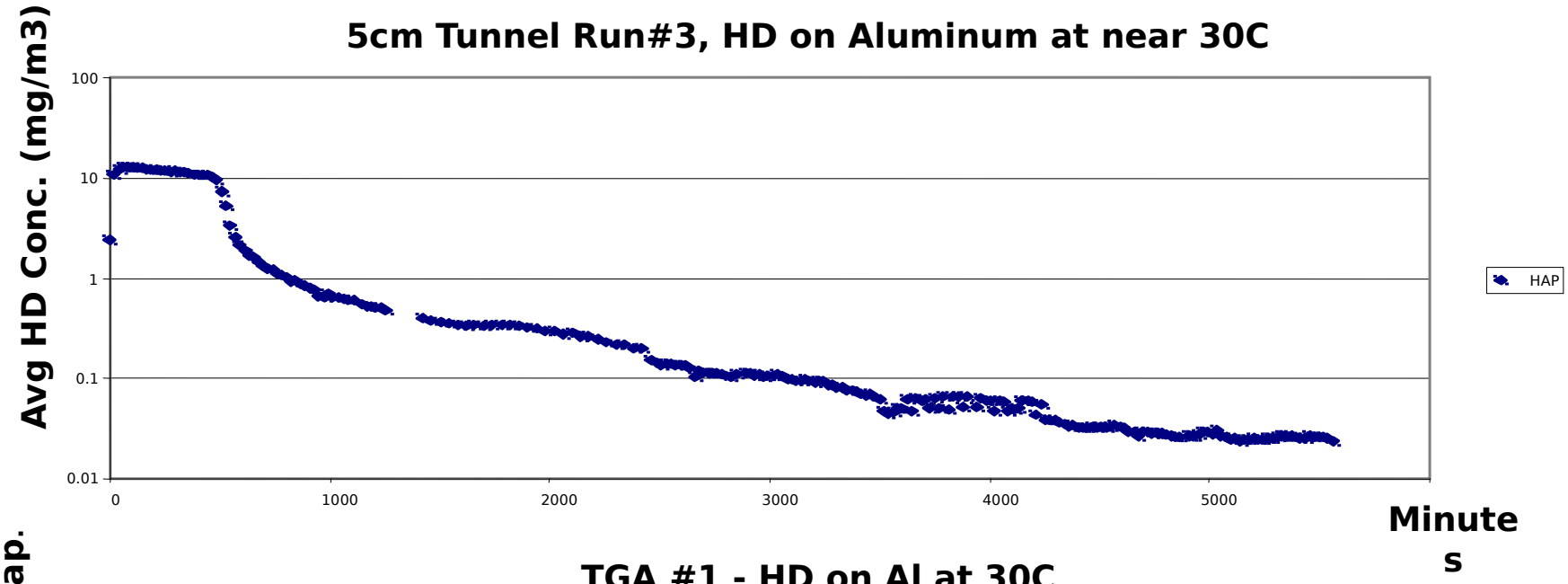
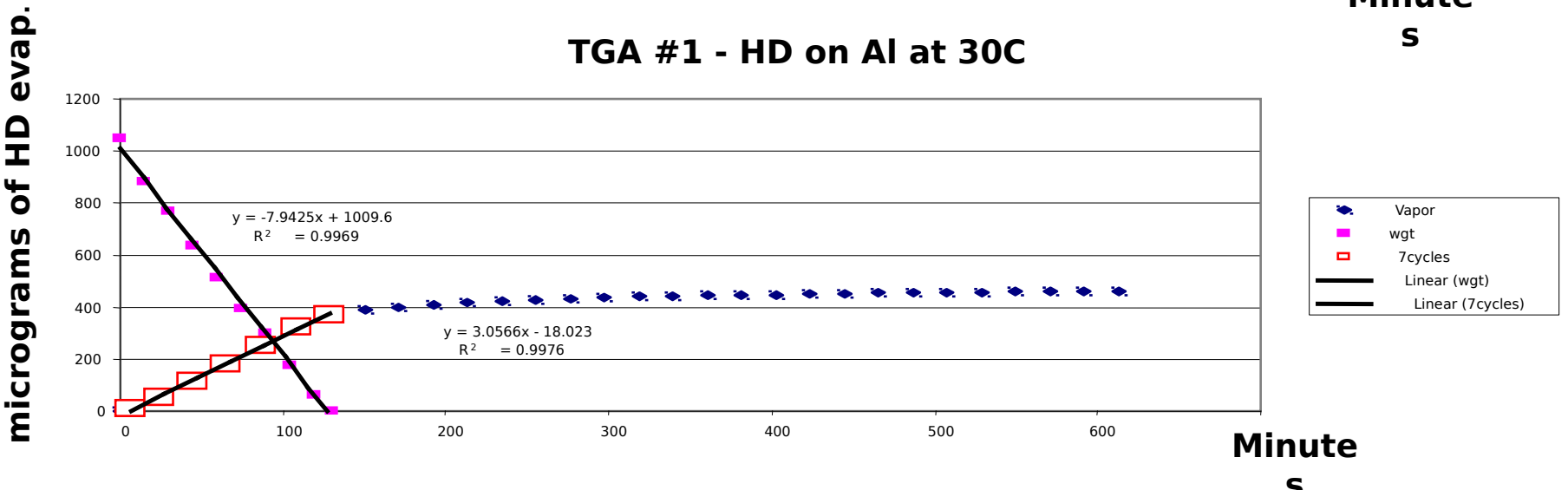
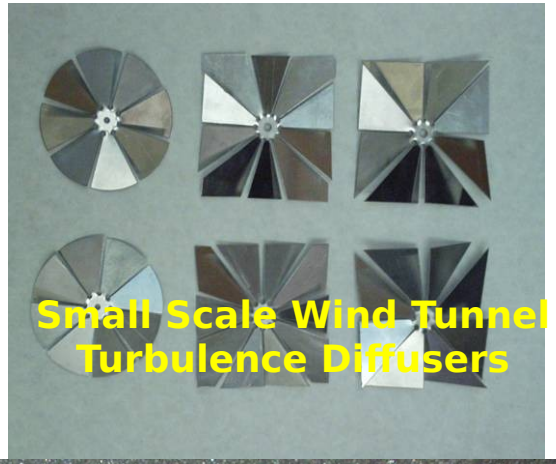

5cm Tunnel Run#3, HD on Aluminum at near 30C
Avg HD Conc. (mg/m3)
100
10
1
0.1
0.01
0
1000
2000
3000
4000
5000
HAP
Minutes


TGA #1 - HD on Al at 30C
micrograms of HD evap.
1200
1000
800
600
400
200
0
y = -7.9425x + 1009.6
R² = 0.9969
y = 3.0566x - 18.023
R² = 0.9976
0
100
200
300
400
500
600
Vapor
wgt
7cycles
Linear (wgt)
Linear (7cycles)
Minutes

Where We Are Today
Wind Tunnel

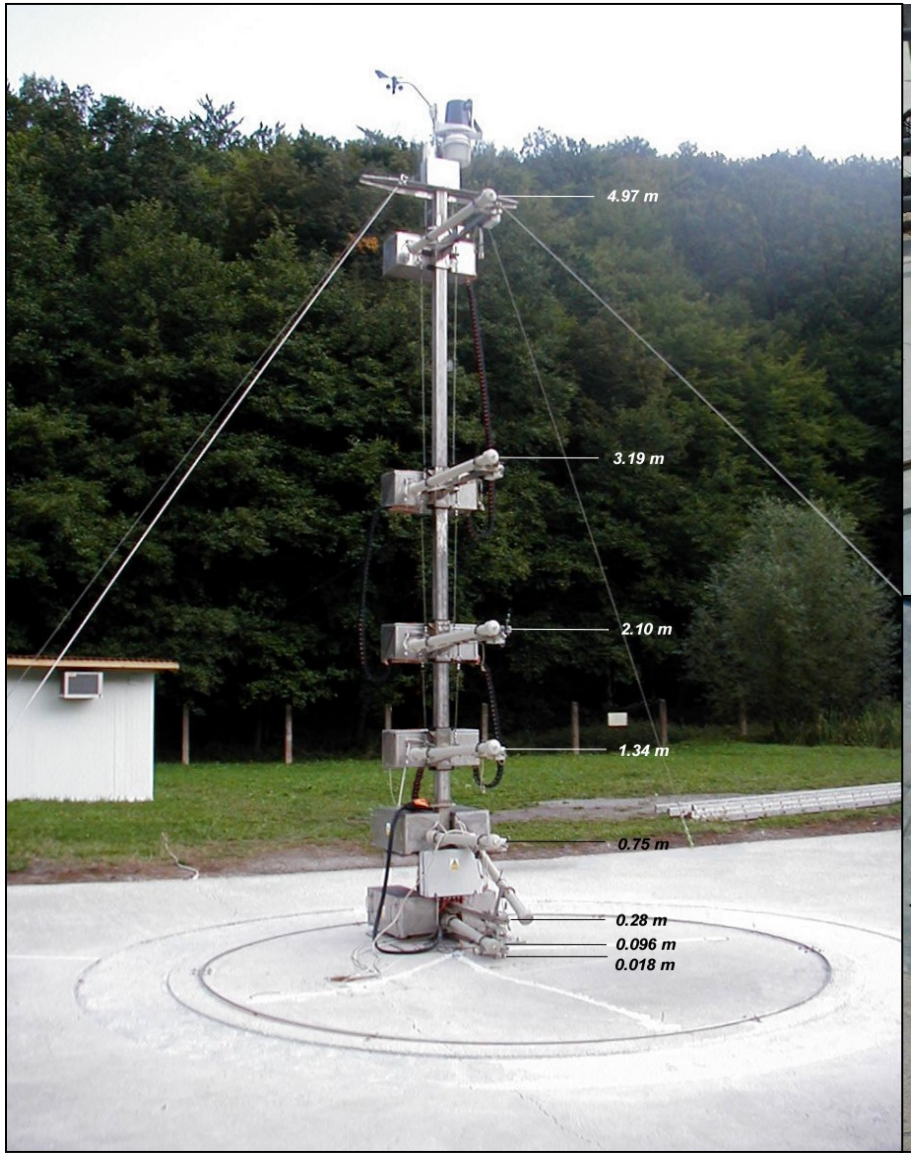
Small Scale Wind Tunnel

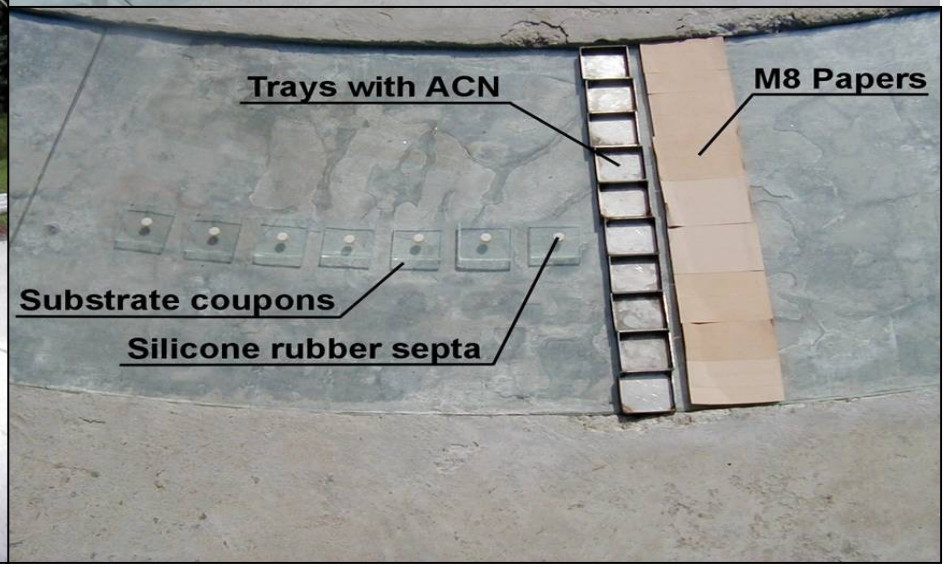

Small Scale Wind Tunnel
Turbulence Diffusers

Large Scale Wind Tunnel

Small Scale Wind Tunnel

Where We Are Today
Czech Outdoor Test Facilities





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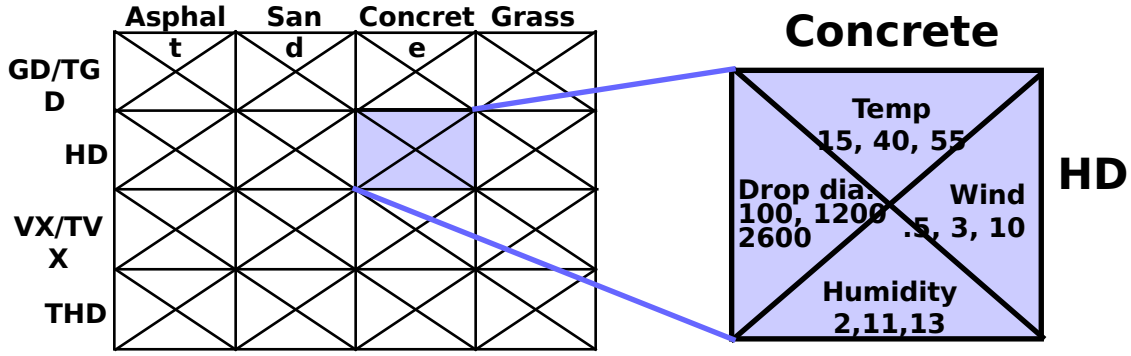
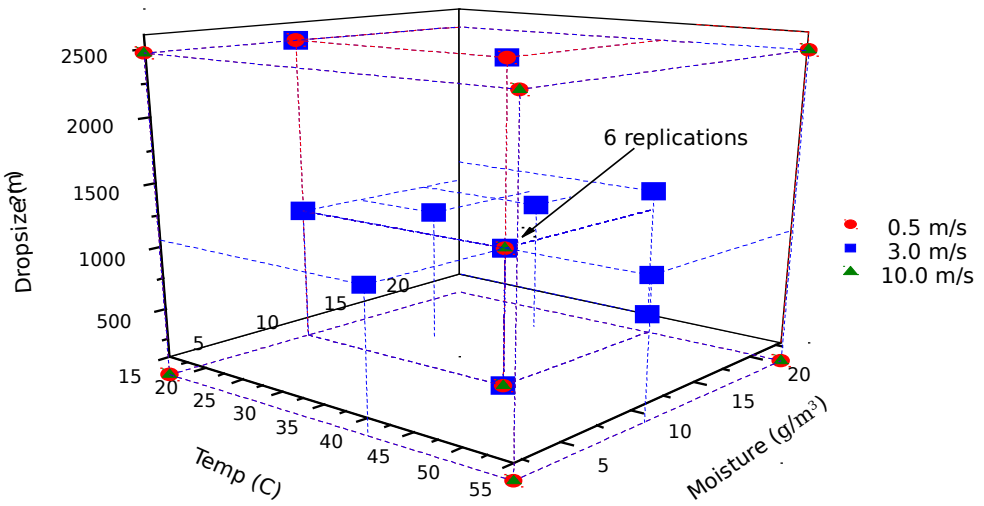
Thrust: Predictive Modeling

- Created central composite design (CCD) experimental test matrix
- Developed surface evaporation assessment tool
- Incorporated 26,115 new data elements into evaporation database
- Completed phase II literature analysis
- Fielded CHEMRAT phase I



- About 10,000 experiments for full factorial approach – infeasible!
- Now, about 1500 experiments with CCD approach
  - 24 agent/substrate combinations
  - 3 levels for each parameter (temp., drop dia., wind speed, humidity)

HD on Concrete CCD Experiments



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Why Do We Need Better Agent Fate Models?

Field manuals and models built from limited data sets & questionable FY03 data Products

- **Methodology Development – VX fate on concrete**
- **Lab/Wind Tunnel – Validated tunnel designs**
- **Predictive Modeling – CHEMRAT phase I; Statistically optimized test matrix**

Concrete/Asphalt		FM 3-4		FM 3-3/ FM 3-7		FM 3-9		CONOPS	
	Temp	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor
GD	10-30ºC	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	<0.2	.5 - 6
HD	10-30ºC	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	<0.2	1 - 4.5
VX	10-30ºC	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	<0.2	1 - 7.5

Sand		FM 3-4		FM 3-3/ FM 3-7		FM 3-9		CONOPS	
	Temp	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor
GD	10-30ºC	Not Avail	18 - 60+	Not Avail	11 - 44	Not Avail	5 - 48	<0.2	.5 - 5
HD	10-30ºC	Not Avail	60+	Not Avail	3 - 12	Not Avail	6 - 168	<0.2	.5 - 4
VX	10-30ºC	Not Avail	45 - 60+	Not Avail	1085 - 7992	Not Avail	1800 -3600	<0.2	7.5 - 10

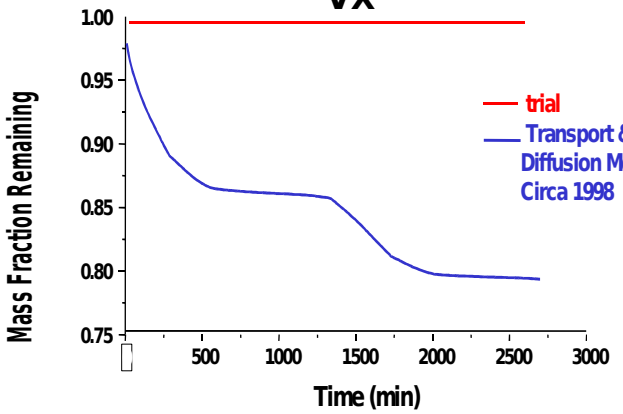
Grass		FM 3-4		FM 3-3/ FM 3-7		FM 3-9		CONOPS	
	Temp	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor
GD	10-30ºC	Not Avail	7 - 20+	Not Avail	4-17	Not Avail	5 - 48	4*	.5 - 5
HD	10-30ºC	Not Avail	20+	Not Avail	1 - 5	Not Avail	6 - 168	4*	.5 - 4
VX	10-30ºC	Not Avail	18 - 20+	Not Avail	422 -3108	Not Avail	1800 -3600	4*	7.5 - 10

FM 3-4

Temp 10-30 C	Liquid	Vapor
GD	Not Avail	7 - 20+
HD	Not Avail	20+
VX	Not Avail	18 - 20+

FM 3-9

Temp 10-30 C	Liquid	Vapor
GD	Not Avail	5 - 48
HD	Not Avail	6 - 168
VX	Not Avail	1800 -3600



Why not just better Tables?

- Available hazard persistence tables/charts are inconsistent
  - Wide variations in persistence times
- Many reasons for these wide variations:
  - Different definitions of hazard
  - Limited ability to predict residual vapor challenge
  - Different threat weapon systems and agents considered
  - Inability to communicate random effects (statistical variations) for:
    - Weather
    - Weapon CEP and performance
    - Variation of hot spot locations

Further Limitations with Tables

- Including these variations in hazard charts results in
  - Voluminous tables of numbers,
  - Pages of caveats, and,
  - Results that are difficult to understand
- Requires tables to be generated for each specific case
  - Threat type (weapon, agent, dissemination type)
  - Weather condition
  - Casualty level (lethal, incapacitation, threshold)
  - Exposure (duration, route of entry, protection)
  - Risk level (most sensitive person, average person, etc.)
    - Casualty probability (1 % chance, 10% chance,…)
- Tables cannot be used to examine trade-offs between risk, exposure, and persistence time

Examples of User Questions

- How long do I have to wait until I can be 99% certain that my most sensitive people will not receive an incapacitation one hour no-mask exposure?
- How long do I have to wait until I can be 90% certain that people (say 95% of my people) can work a 12 hour shift without a mask and not receive a miosis exposure?
- I've just been attacked, and I've got to do 5 hours of work to accomplish my mission. What is the risk to my population of receiving a lethal exposure?

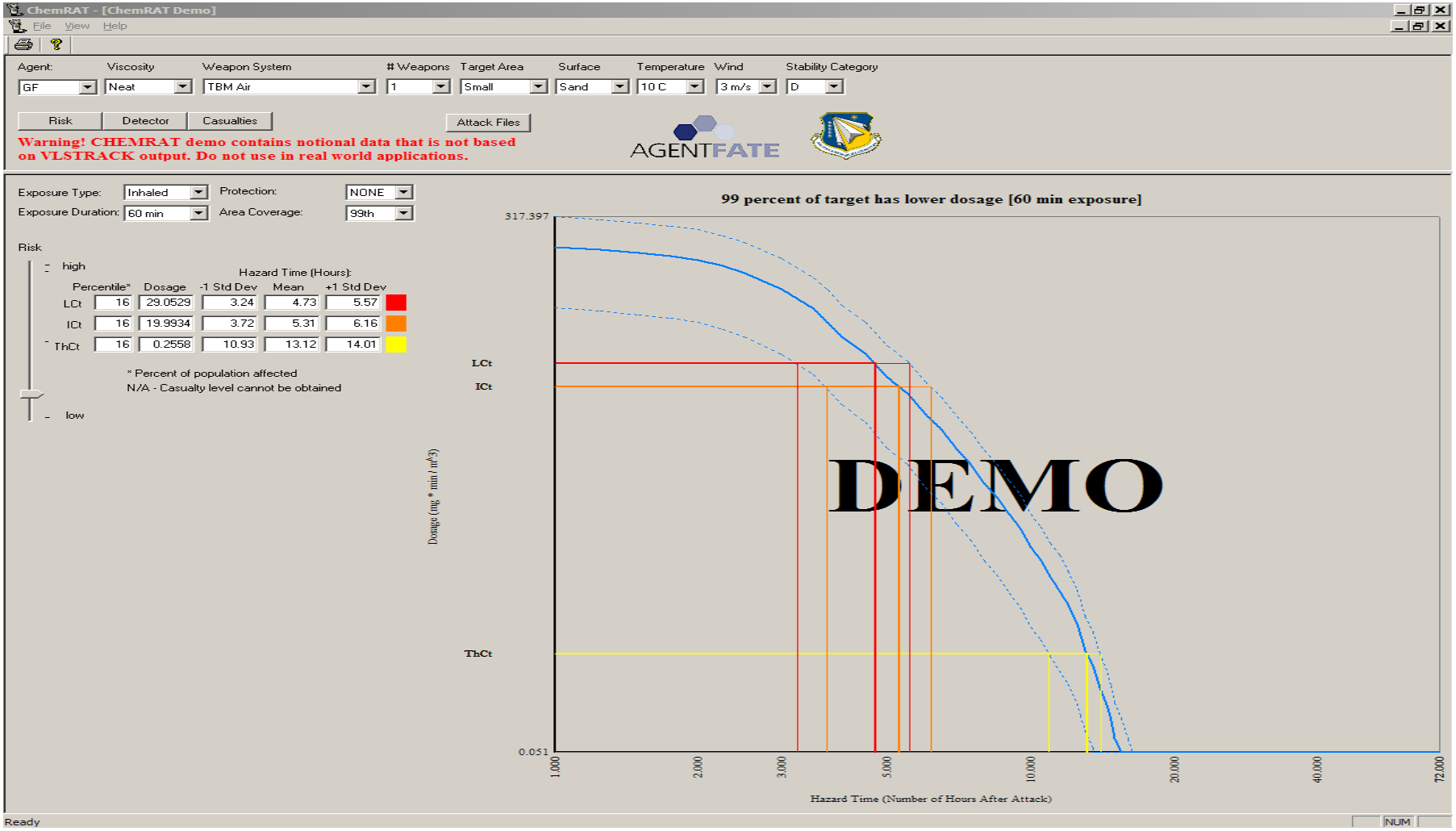
Example : Interpretation

GF filled TBM attack, 1 missile, 10C, 3m/s on Sand, small target, 99th percentile vapor coverage (worst 1% on the target), 60 minute inhalation exposure duration, no mask

- For people standing at the base location having the 99th percentile vapor concentration (worst 1% of the base)
  - 16 % of these people will be effected by exposures of
    - .26 mg min/m^3 for threshold effects (miosis)
    - 19.99 mg min/m^3 for severe incapacitation effects
    - 29.05 mg min/m^3 for lethal effects
  - These are the more susceptible members of the population, 84% of the people at the same location will require higher exposures for the same effects
- Threshold level hazard is expected to persist for about 14 hours (11.8 – 14.5 hours)*
- Severe incapacitation level hazard is expected to persist for about 6 hours*
- Lethal level hazard is expected to persist for about 5.4 hours*

**Notional Data – Not to be used for real world applications*

THE ANSWER


ChemRAT - [ChemRAT Demo]
File View Help
Agent: GF
Viscosity: Neat
Weapon System: TBM Air
Weapons: 1
Target Area: Small
Surface: Sand
Temperature: 10 C
Wind: 3 m/s
Stability Category: D
Risk
Detector
Casualties
Attack Files
Warning! CHEMRAT demo contains notional data that is not based on VLSTRACK output. Do not use in real world applications.
AGENTFATE
Exposure Type: Inhaled
Protection: NONE
Exposure Duration: 60 min
Area Coverage: 99th
Risk
high
low
Hazard Time (Hours):
Percentile* Dosage -1 Std Dev Mean +1 Std Dev
LCt 16 29.0529 3.24 4.73 5.57
ICt 16 19.9934 3.72 5.31 6.16
ThCt 16 0.2558 10.93 13.12 14.01
* Percent of population affected
N/A - Casualty level cannot be obtained
99 percent of target has lower dosage [60 min exposure]
317.397
LCt
ICt
ThCt
0.051
Dosage (mg * min / m^3)
DEMO
1.000
2.000
3.000
5.000
10.000
20.000
40.000
72.000
Hazard Time (Number of Hours After Attack)
Ready
NUM

Risk Assessment Tool

CHEMRAT displays answers to these questions in a graphical manner so that sensitivities can be investigated and inferred by the warfighter

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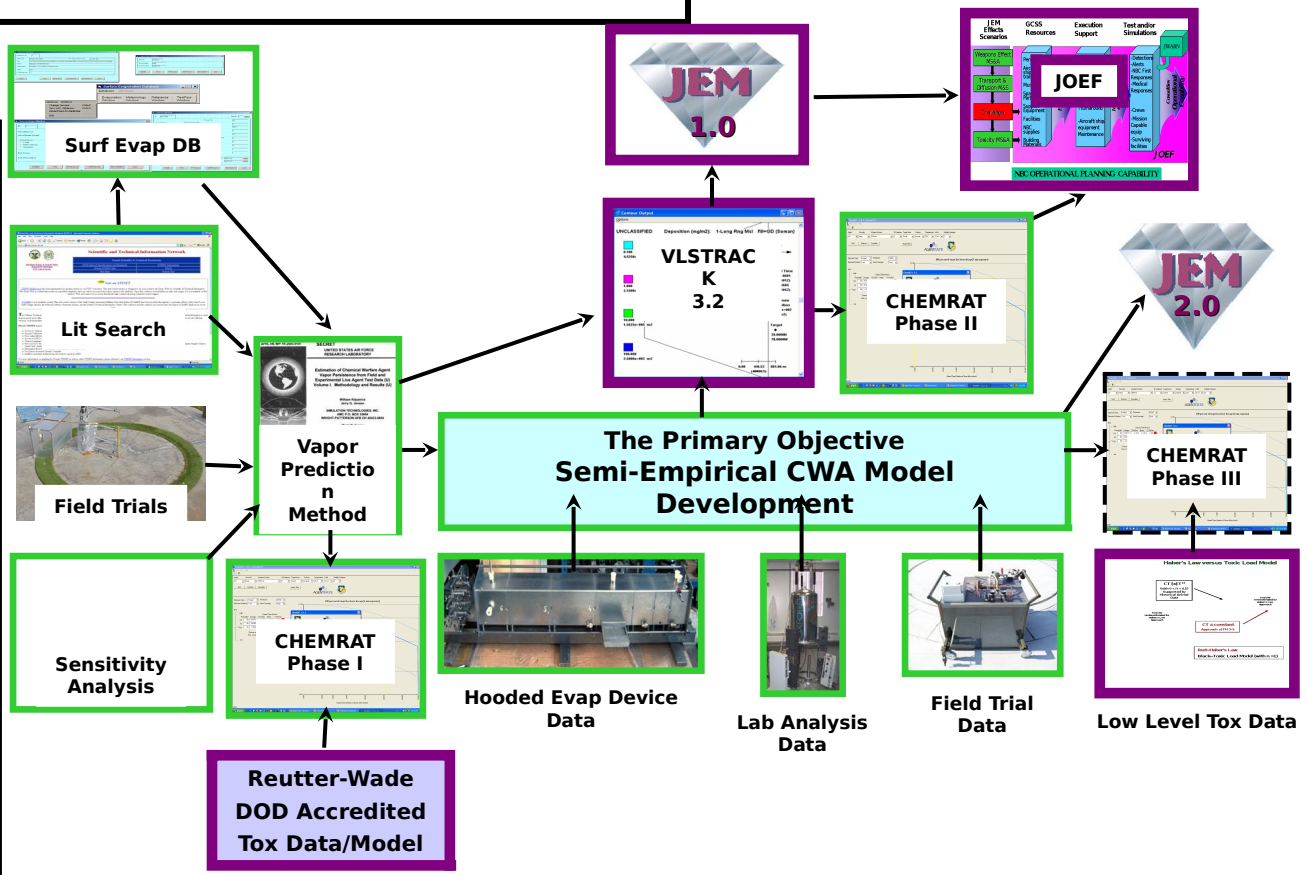
Thrust: Predictive Modeling Development

Surface Evap Model

- Data Scaling
- Sensitivity Analysis
- Literature Survey
- Surface Evap Database Expansion & Upgrade

Interim Prediction Tools

- VLSTRACK Upgrade
- CHEMRAT 1 & 2



Questions

"Both Communities *{AF Bioenvironmental Engineering and CE Readiness Career fields}* agreed that CHEMRAT is a highly valuable tool that will greatly enhance the AF ability to survive and operated in a CW environment." *HQ USAF/SGX ltr dtd Jan 06, 2003*

Joseph E. Kelly, Brigadier General, USAF, MC, CFS